

FULL ESTIMATED COST

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FILE COVERS 1907 - 20 Sep 2004 VOL 141 ISS 13
 FILE LAST UPDATED: 19 Sep 2004 (20040919/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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=> s raf {} kinase
      5313 RAF
      52 RAFS
      5346 RAF
          (RAF OR RAFS)
      223150 KINASE
      44622 KINASES
      230583 KINASE
          (KINASE OR KINASES)
L1      784 RAF (W) KINASE

=> s l1 and inhibitor?
      894275 INHIBITOR?
L2      347 L1 AND INHIBITOR?

=> s l2 and carcinoma? {} lung?
      122251 CARCINOMA?
      172706 LUNG?
      333 CARCINOMA? (W) LUNG?
L3      0 L2 AND CARCINOMA? (W) LUNG?

=> s l2 and carcinoma?
      122251 CARCINOMA?
L4      32 L2 AND CARCINOMA?

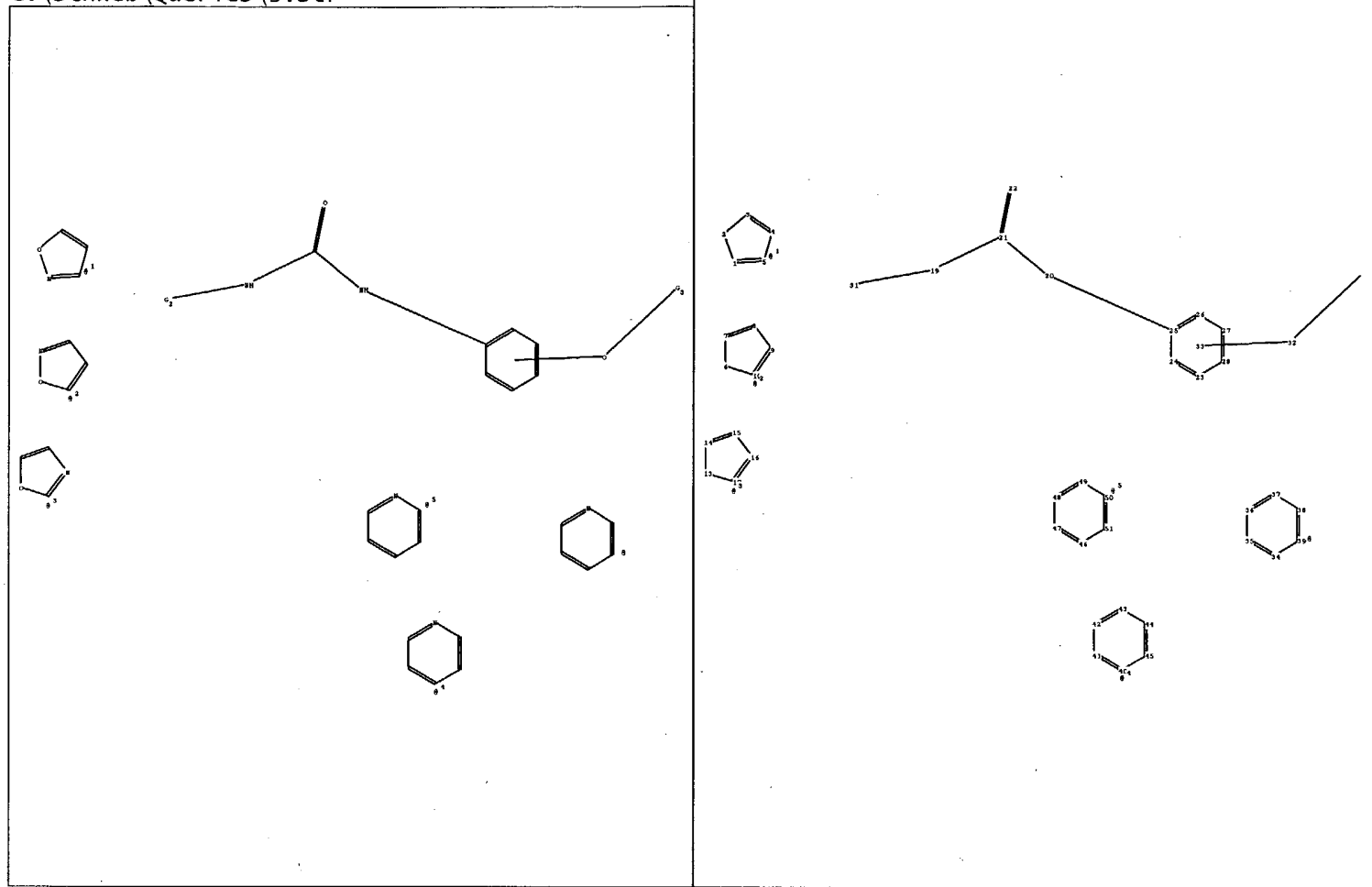
=> s l4 and review/dt
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L5      1 L4 AND REVIEW/DT

=> d l5, ibib abs, 1

L5      ANSWER 1 OF 1 HCAPLUS  COPYRIGHT 2004 ACS on STN
```

Full Text	Query References
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ACCESSION NUMBER: 2003:736198 HCAPLUS



chain nodes :

19 20 21 22 31 32 58

ring nodes :

1 2 3 4 5 6 7 8 9 10 13 14 15 16 17 23 24 25 26 27 28 34 35 36 37
38 39 40 41 42 43 44 45 46 47 48 49 50 51

chain bonds :

19-21 19-31 20-21 20-25 21-22 32-58

ring bonds :

1-2 1-5 2-3 3-4 4-5 6-7 6-10 7-8 8-9 9-10 13-14 13-17 14-15 15-16 16-17
23-24 23-28 24-25 25-26 26-27 27-28 34-35 34-39 35-36 36-37 37-38 38-39 40-41
40-45 41-42 42-43 43-44 44-45 46-47 46-51 47-48 48-49 49-50 50-51

exact/norm bonds :

1-5 7-8 15-16 16-17 19-21 19-31 20-21 20-25 21-22 32-58

exact bonds :

1-2 2-3 3-4 4-5 6-7 6-10 8-9 9-10 13-14 13-17 14-15

normalized bonds :

23-24 23-28 24-25 25-26 26-27 27-28 34-35 34-39 35-36 36-37 37-38 38-39 40-41
40-45 41-42 42-43 43-44 44-45 46-47 46-51 47-48 48-49 49-50 50-51

isolated ring systems :

containing 1 : 6 : 13 : 23 : 34 : 40 : 46 :

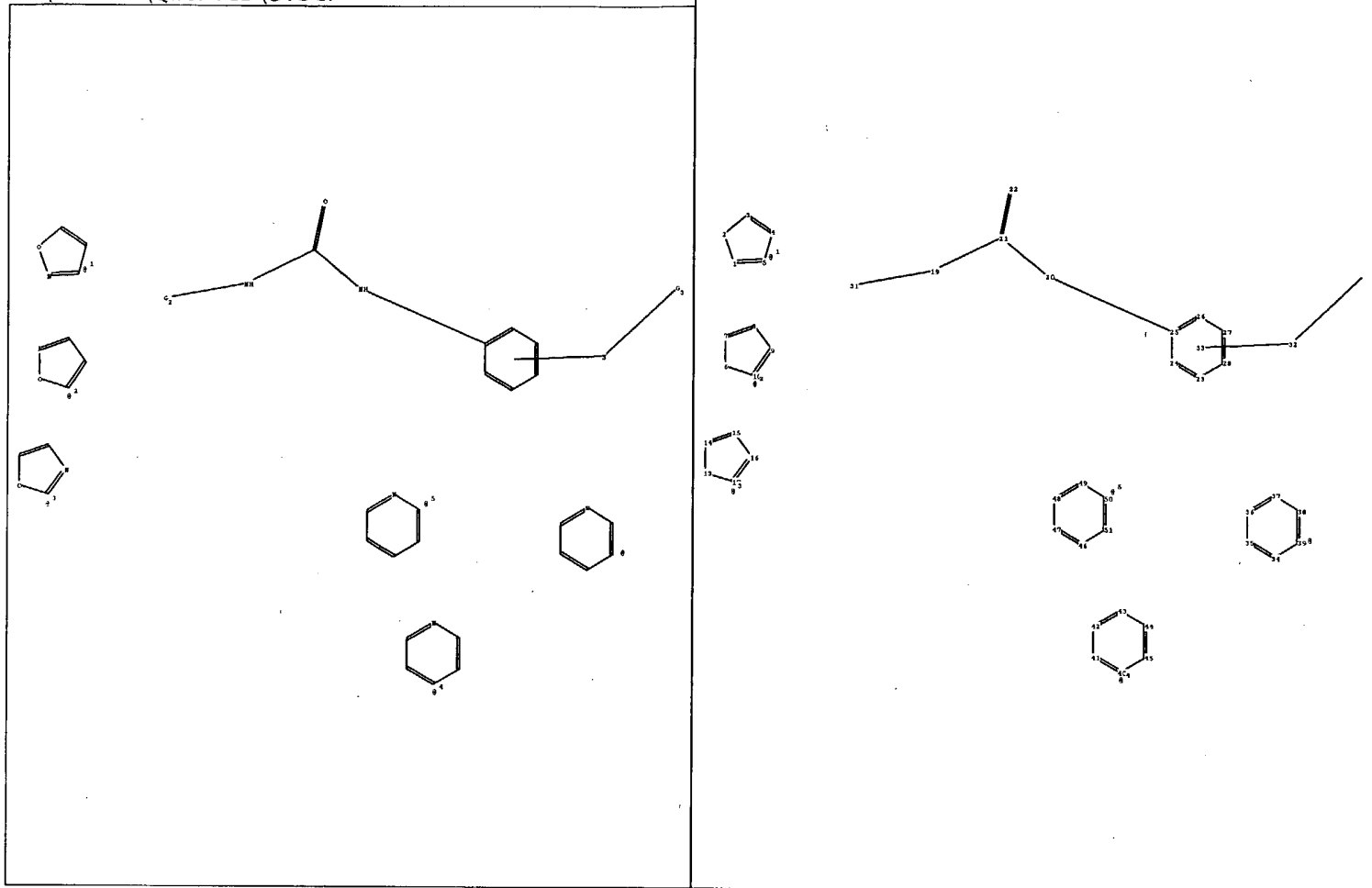
G1:O,S

G2:[*1],[*2],[*3]

G3:Ph,[*4],[*5]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 13:Atom
14:Atom 15:Atom 16:Atom 17:Atom 19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:Atom
24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 31:CLASS 32:CLASS 33:CLASS 34:Atom
35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom 42:Atom 43:Atom 44:Atom
45:Atom 46:Atom 47:Atom 48:Atom 49:Atom 50:Atom 51:Atom 58:CLASS



chain nodes :

19 20 21 22 31 32 58

ring nodes :

1 2 3 4 5 6 7 8 9 10 13 14 15 16 17 23 24 25 26 27 28 34 35 36 37
38 39 40 41 42 43 44 45 46 47 48 49 50 51

chain bonds :

19-21 19-31 20-21 20-25 21-22 32-58

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1-2 1-5 2-3 3-4 4-5 6-7 6-10 7-8 8-9 9-10 13-14 13-17 14-15 15-16 16-17
23-24 23-28 24-25 25-26 26-27 27-28 34-35 34-39 35-36 36-37 37-38 38-39 40-41
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1-5 7-8 15-16 16-17 19-21 19-31 20-21 20-25 21-22 32-58

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containing 1 : 6 : 13 : 23 : 34 : 40 : 46 :

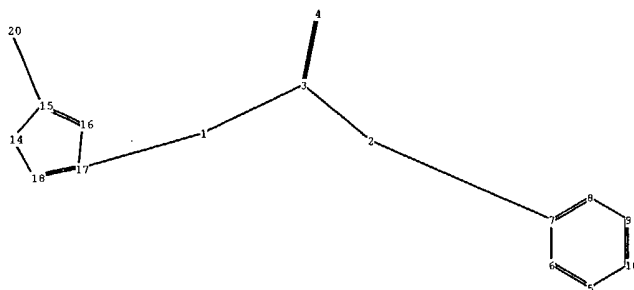
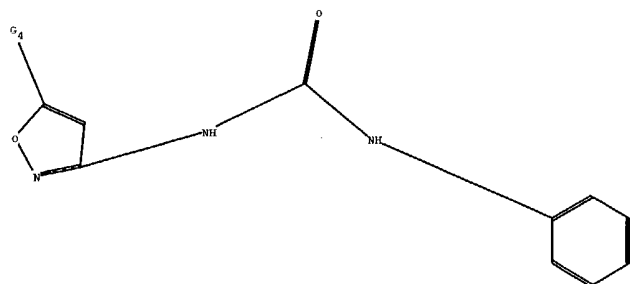
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14:Atom 15:Atom 16:Atom 17:Atom 19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:Atom
24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 31:CLASS 32:CLASS 33:CLASS 34:Atom
35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom 42:Atom 43:Atom 44:Atom
45:Atom 46:Atom 47:Atom 48:Atom 49:Atom 50:Atom 51:Atom 58:CLASS



chain nodes :

1 2 3 4 20

ring nodes :

5 6 7 8 9 10 14 15 16 17 18

chain bonds :

1-3 1-17 2-3 2-7 3-4 15-20

ring bonds :

5-6 5-10 6-7 7-8 8-9 9-10 14-15 14-18 15-16 16-17 17-18

exact/norm bonds :

1-3 1-17 2-3 2-7 3-4 14-15 14-18 15-16 15-20 16-17 17-18

normalized bonds :

5-6 5-10 6-7 7-8 8-9 9-10

G1:O,S

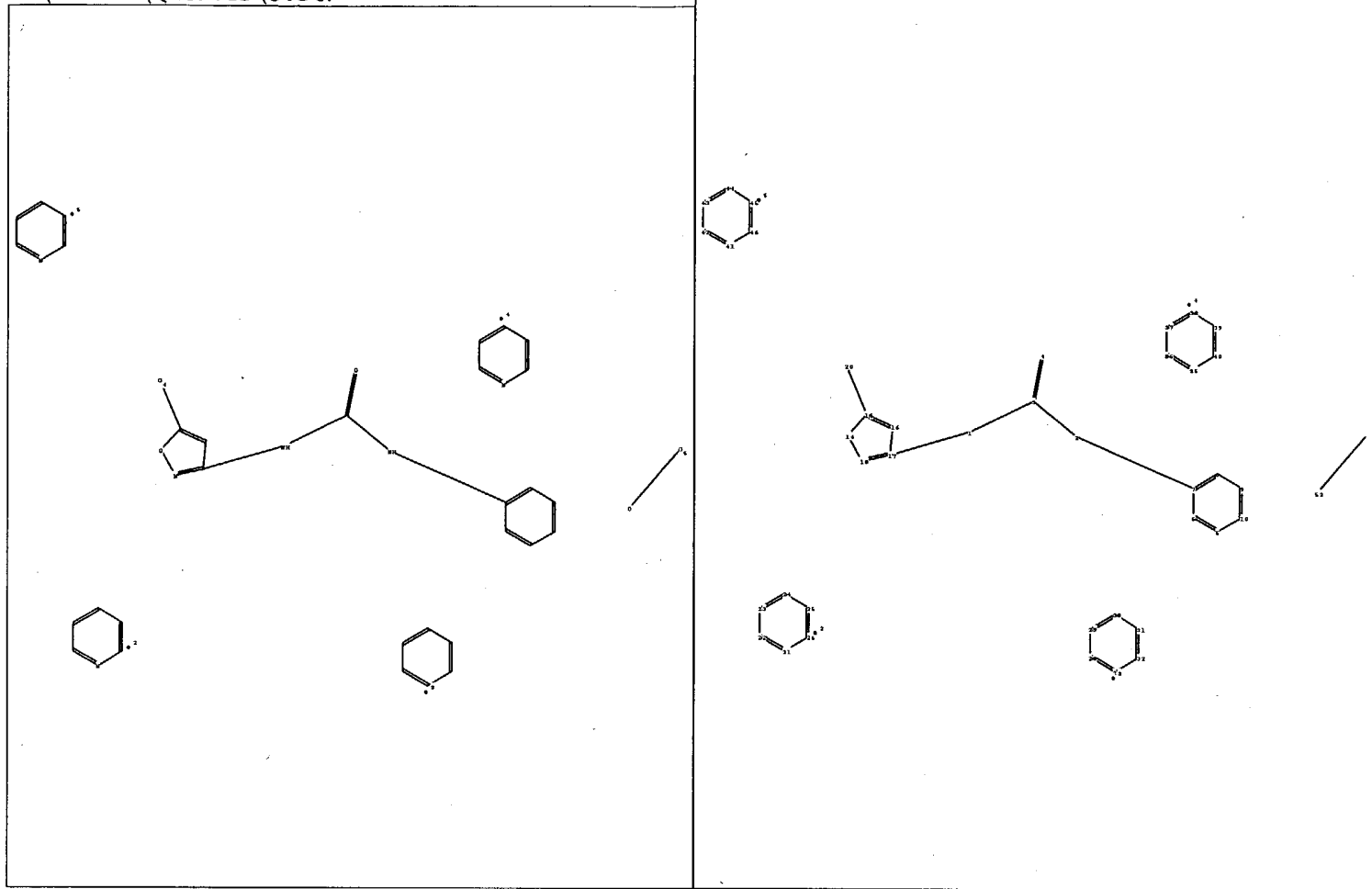
G2

G3:Ph

G4:Cb,Ak

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 20:CLASS



chain nodes :

1 2 3 4 20 51 52

ring nodes :

5 6 7 8 9 10 14 15 16 17 18 21 22 23 24 25 26 27 28 29 30 31 32 35
36 37 38 39 40 41 42 43 44 45 46

chain bonds :

1-3 1-17 2-3 2-7 3-4 15-20 51-52

ring bonds :

5-6 5-10 6-7 7-8 8-9 9-10 14-15 14-18 15-16 16-17 17-18 21-22 21-26 22-23
23-24 24-25 25-26 27-28 27-32 28-29 29-30 30-31 31-32 35-36 35-40 36-37 37-38
38-39 39-40 41-42 41-46 42-43 43-44 44-45 45-46

exact/norm bonds :

1-3 1-17 2-3 2-7 3-4 15-20 17-18 51-52

exact bonds :

14-15 14-18 15-16 16-17

normalized bonds :

5-6 5-10 6-7 7-8 8-9 9-10 21-22 21-26 22-23 23-24 24-25 25-26 27-28 27-32
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43-44 44-45 45-46

isolated ring systems :

containing 5 : 14 : 21 : 27 : 35 : 41 :

G1:O,S

G2

G3:Ph

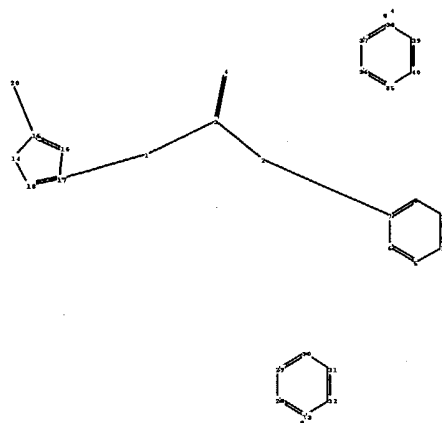
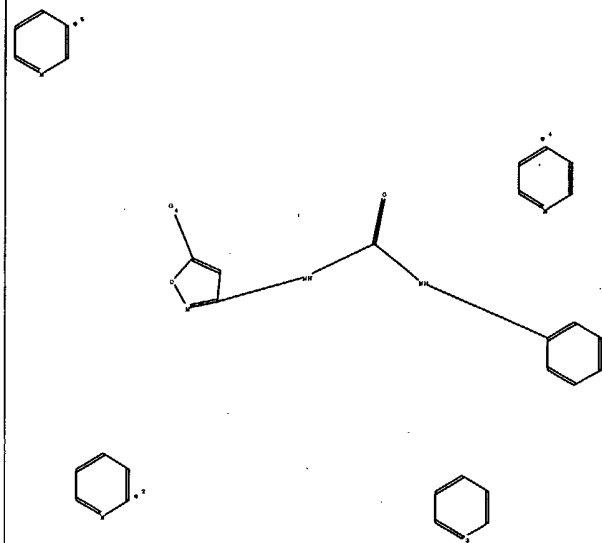
G4:Cb,Ak

G5:[*2],[*3],[*4],[*5]

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 20:CLASS 21:Atom 22:Atom 23:Atom 24:Atom
25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom 32:Atom 35:Atom 36:Atom
37:Atom 38:Atom 39:Atom 40:Atom 41:Atom 42:Atom 43:Atom 44:Atom 45:Atom 46:Atom
51:CLASS 52:CLASS

C:\stnweb\Queries\8.str



chain nodes :

1 2 3 4 20 51 52

ring nodes :

5 6 7 8 9 10 14 15 16 17 18 21 22 23 24 25 26 27 28 29 30 31 32 35
36 37 38 39 40 41 42 43 44 45 46

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1-3 1-17 2-3 2-7 3-4 15-20 51-52

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1-3 1-17 2-3 2-7 3-4 15-20 17-18 51-52

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G2

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25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom 32:Atom 35:Atom 36:Atom
37:Atom 38:Atom 39:Atom 40:Atom 41:Atom 42:Atom 43:Atom 44:Atom 45:Atom 46:Atom
51:CLASS 52:CLASS

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<u>NEWS 4</u>	May 12	Polymer links for the POLYLINK command completed in REGISTRY
<u>NEWS 5</u>	May 27	New UPM (Update Code Maximum) field for more efficient patent SDIs in CAplus
<u>NEWS 6</u>	May 27	CAplus super roles and document types searchable in REGISTRY
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<u>NEWS 12</u>	AUG 02	CAplus and CA patent records enhanced with European and Japan Patent Office Classifications
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<u>NEWS 17</u>	AUG 27	BIOTECHABS/BIOTECHDS: Two new display fields added for legal status data from INPADOC
<u>NEWS 18</u>	SEP 01	INPADOC: New family current-awareness alert (SDI) available
<u>NEWS 19</u>	SEP 01	New pricing for the Save Answers for SciFinder Wizard within STN Express with Discover!
<u>NEWS 20</u>	SEP 01	New display format, HITSTR, available in WPIDS/WPINDEX/WPIX
<u>NEWS 21</u>	SEP 14	STN Patent Forum to be held October 13, 2004, in Iselin, NJ
<u>NEWS EXPRESS</u>	JULY 30	CURRENT WINDOWS VERSION IS V7.01, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 11 AUGUST 2004
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=> file hcplus

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=> file hcaplus

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SINCE FILE

TOTAL

ENTRY

SESSION

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eb

FULL ESTIMATED COST

0.21

0.21

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=> s l4 and review/dt
      1758970 REVIEW/DT
L5      1 L4 AND REVIEW/DT

=> d l5, ibib abs, 1

L5 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN
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Full Text	Citing References
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ACCESSION NUMBER: 2003:736198 HCAPLUS

DOCUMENT NUMBER: 139:301125
 TITLE: BAY-43-9006 (Bayer/Onyx)
 AUTHOR(S): Lee, John T.; McCubrey, James A.
 CORPORATE SOURCE: Department of Microbiology and Immunology, Brody
 School of Medicine at East Carolina University,
 Greenville, NC, 27858-4353, USA
 SOURCE: Current Opinion in Investigational Drugs (Thomson
 Current Drugs) (2003), 4(6), 757-763
 CODEN: COIDAZ; ISSN: 1472-4472
 PUBLISHER: Thomson Current Drugs
 DOCUMENT TYPE: Journal; **General Review**
 LANGUAGE: English
 AB A review. Bayer and Onyx are developing BAY-43-9006, an oral cytostatic
Raf kinase inhibitor for the potential treatment of colorectal and
 breast cancers, hepatocellular **carcinoma** and non-small-cell lung cancer,
 in addn. to acute myelogenous leukemia, myelodysplastic syndrome and other
 cancers. A US IND was filed in May 2000 and by Feb. 2003 BAY-43-9006 was
 in phase II trials, with phase III trials expected to begin later in 2003.
 REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d his

(FILE 'HOME' ENTERED AT 14:48:16 ON 20 SEP 2004)

FILE 'HCAPLUS' ENTERED AT 14:48:22 ON 20 SEP 2004

L1 784 S RAF () KINASE
 L2 347 S L1 AND INHIBITOR?
 L3 0 S L2 AND CARCINOMA? () LUNG?
 L4 32 S L2 AND CARCINOMA?
 L5 1 S L4 AND REVIEW/DT

=> s l2 and adenoma?
 13502 ADENOMA?

L6 2 L2 AND ADENOMA?

=> s l6 and review/dt
 1758970 REVIEW/DT
 L7 0 L6 AND REVIEW/DT

=> s l2 and cancer?
 236073 CANCER?
 L8 108 L2 AND CANCER?

=> s l8 and lung?
 172706 LUNG?
 L9 29 L8 AND LUNG?

=> s l9 and review/dt
 1758970 REVIEW/DT
 L10 3 L9 AND REVIEW/DT

=> d l10, ibib abs, 1-3

L10 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text Citations
 References

ACCESSION NUMBER: 2004:309398 HCAPLUS
 DOCUMENT NUMBER: 141:21179

TITLE: **Raf kinase inhibitor** protein: a prostate **cancer** metastasis suppressor gene
 AUTHOR(S): Keller, Evan T.; Fu, Zheng; Yeung, Kam; Brennan, Meghan
 CORPORATE SOURCE: Department of Urology, University of Michigan, Ann Arbor, MI, 48109-0940, USA
 SOURCE: Cancer Letters (Amsterdam, Netherlands) (2004), 207(2), 131-137
 CODEN: CALEDQ; ISSN: 0304-3835
 PUBLISHER: Elsevier
 DOCUMENT TYPE: Journal; **General Review**
 LANGUAGE: English

AB A review. Defining the mechanisms that confer metastatic ability on **cancer** cells is an important goal towards prevention of metastasis. A gene array screen between a non-metastatic prostate **cancer** cell and its metastatic deriv. line revealed decreased expression of **Raf kinase inhibitor** protein (RKIP) in the metastatic cell line. This finding is consistent with the possibility that loss of RKIP is assocd. with metastasis. RKIP is expressed in many tissues including brain, **lung**, and liver. RKIP blocks Raf-induced phosphorylation of MEK. In addn. to its modulation of Raf signaling, RKIP modulates both G-protein signaling and NF- κ B activity. The impact that RKIP has on multiple signaling pathways grants it the ability to play a role in several cellular functions including membrane biosynthesis, spermatogenesis, and neural signaling. Novel cellular functions for RKIP continue to be identified, several of which contribute to **cancer** biol. For example, RKIP promotes apoptosis of **cancer** cells, which suggests that loss of RKIP in **cancer** will protect **cancer** cells against cell death. Addnl., restoration of RKIP expression in a metastatic prostate **cancer** cell line does not effect primary tumor growth, but it does inhibit prostate **cancer** metastasis. These parameters identify RKIP as a metastasis suppressor gene, which suggest that it or proteins it interacts are putative mol. targets to control metastasis. These findings are supported by the observation that RKIP expression is decreased in metastases of prostate **cancer** patients, compared to normal prostate or the primary prostate tumor. In this review, RKIP biol. and its role in **cancer** will be described.

REFERENCE COUNT: 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text	References
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ACCESSION NUMBER: 2003:736198 HCAPLUS
 DOCUMENT NUMBER: 139:301125
 TITLE: BAY-43-9006 (Bayer/Onyx)
 AUTHOR(S): Lee, John T.; McCubrey, James A.
 CORPORATE SOURCE: Department of Microbiology and Immunology, Brody School of Medicine at East Carolina University, Greenville, NC, 27858-4353, USA
 SOURCE: Current Opinion in Investigational Drugs (Thomson Current Drugs) (2003), 4(6), 757-763
 CODEN: COIDAZ; ISSN: 1472-4472
 PUBLISHER: Thomson Current Drugs
 DOCUMENT TYPE: Journal; **General Review**
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AB A review. Bayer and Onyx are developing BAY-43-9006, an oral cytostatic **Raf kinase inhibitor** for the potential treatment of colorectal and breast **cancers**, hepatocellular carcinoma and non-small-cell **lung cancer**, in addn. to acute myelogenous leukemia, myelodysplastic syndrome

and other **cancers**. A US IND was filed in May 2000 and by Feb. 2003 BAY-43-9006 was in phase II trials, with phase III trials expected to begin later in 2003.

REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text 

ACCESSION NUMBER: 2002:363470 HCAPLUS
DOCUMENT NUMBER: 137:229993
TITLE: The role of **Raf kinases** in malignant transformation
AUTHOR(S): Kolch, Walter; Kotwaliwale, Ashwin; Vass, Keith; Janosch, Petra
CORPORATE SOURCE: Institute for Biomedical and Life Sciences, University of Glasgow, Glasgow, G12 8QQ, UK
SOURCE: Expert Reviews in Molecular Medicine [online computer file] (2002) No pp. given
CODEN: ERMMS; ISSN: 1462-3994
URL: <http://www.expertreviews.org/02004386a.pdf>
PUBLISHER: Cambridge University Press
DOCUMENT TYPE: Journal; **General Review**; (online computer file)
LANGUAGE: English

AB A review. The **Raf kinases** are proto-oncogenes that work at the entry point of the mitogen-activated protein kinase/extracellular-signal-regulated kinase (MAPK/ERK) pathway, a signalling module that connects cell-surface receptors and Ras proteins to nuclear transcription factors. The pathway impinges on all the functional hallmarks of **cancer** cells: immortalization, growth-factor-independent proliferation, insensitivity to growth-inhibitory signals, ability to invade and metastasize, ability to attract blood vessels, and evasion of apoptosis. Indeed, the pathway is hyperactivated in 30% of all human tumors including prevalent **cancers** of the colon and lung. The mol. mechanisms underlying the role of **Raf kinase** in tumorigenesis and the opportunities for therapeutic intervention are reviewed in this article.

REFERENCE COUNT: 77 THERE ARE 77 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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(FILE 'HOME' ENTERED AT 14:48:16 ON 20 SEP 2004)

FILE 'HCAPLUS' ENTERED AT 14:48:22 ON 20 SEP 2004

L1 784 S RAF () KINASE
L2 347 S L1 AND INHIBITOR?
L3 0 S L2 AND CARCINOMA? () LUNG?
L4 32 S L2 AND CARCINOMA?
L5 1 S L4 AND REVIEW/DT
L6 2 S L2 AND ADENOMA?
L7 0 S L6 AND REVIEW/DT
L8 108 S L2 AND CANCER?
L9 29 S L8 AND LUNG?
L10 3 S L9 AND REVIEW/DT

=> s l8 not l9

L11 79 L8 NOT L9

=> s l11 and pancreas?

68591 PANCREAS?

h eb c g cg b cg

eb

L12 0 L11 AND PANCREAS?

=> s 12 and thyroid?
76320 THYROID?

L13 10 L2 AND THYROID?

=> s 113 and review/dt
1758970 REVIEW/DT

L14 0 L13 AND REVIEW/DT

=> s 12 and bladder?
29305 BLADDER?

L15 8 L2 AND BLADDER?

=> s 115 and review/dt
1758970 REVIEW/DT

L16 0 L15 AND REVIEW/DT

=> s 12 and colon?/
'COLON?/' IS NOT A VALID FIELD CODE
For a list of field codes for the current file, enter "HELP SFIELDS"
at an arrow prompt (=>).

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130286 COLON?

L17 35 L2 AND COLON?

=> s 117 and review/dt
1758970 REVIEW/DT

L18 1 L17 AND REVIEW/DT

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L18 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text	References
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ACCESSION NUMBER: 2002:363470 HCAPLUS
DOCUMENT NUMBER: 137:229993
TITLE: The role of **Raf kinases** in malignant transformation
AUTHOR(S): Kolch, Walter; Kotwaliwale, Ashwin; Vass, Keith;
Janosch, Petra
CORPORATE SOURCE: Institute for Biomedical and Life Sciences, University
of Glasgow, Glasgow, G12 8QQ, UK
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URL: <http://www.expertreviews.org/02004386a.pdf>
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AB A review. The **Raf kinases** are proto-oncogenes that work at the entry point of the mitogen-activated protein kinase/extracellular-signal-regulated kinase (MAPK/ERK) pathway, a signalling module that connects cell-surface receptors and Ras proteins to nuclear transcription factors. The pathway impinges on all the functional hallmarks of cancer cells: immortalization, growth-factor-independent proliferation, insensitivity to growth-**inhibitory** signals, ability to invade and metastasize, ability to attract blood vessels, and evasion of apoptosis. Indeed, the pathway is hyperactivated in 30% of all human tumors including prevalent cancers of the **colon** and lung. The mol. mechanisms underlying the role of **Raf**

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(FILE 'HOME' ENTERED AT 14:48:16 ON 20 SEP 2004)

FILE 'HCAPLUS' ENTERED AT 14:48:22 ON 20 SEP 2004

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L3      0 S L2 AND CARCINOMA? () LUNG?
L4      32 S L2 AND CARCINOMA?
L5      1 S L4 AND REVIEW/DT
L6      2 S L2 AND ADENOMA?
L7      0 S L6 AND REVIEW/DT
L8      108 S L2 AND CANCER?
L9      29 S L8 AND LUNG?
L10     3 S L9 AND REVIEW/DT
L11     79 S L8 NOT L9
L12     0 S L11 AND PANCREAS?
L13     10 S L2 AND THYROID?
L14     0 S L13 AND REVIEW/DT
L15     8 S L2 AND BLADDER?
L16     0 S L15 AND REVIEW/DT
L17     35 S L2 AND COLON?
L18     1 S L17 AND REVIEW/DT

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=> s l11 not l18

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L19     79 L11 NOT L18

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=> s l19 and myeloid () disorder?

19564 MYELOID

10 MYELOIDS

19567 MYELOID

(MYELOID OR MYELOIDS)

380301 DISORDER?

125 MYELOID (W) DISORDER?

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L20     0 L19 AND MYELOID (W) DISORDER?

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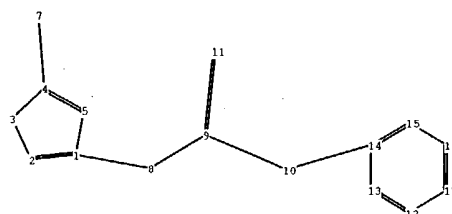
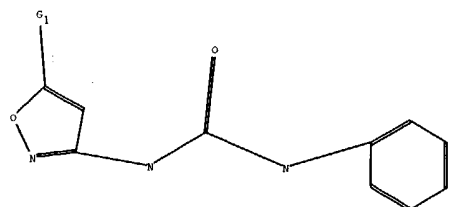
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DOCUMENT NUMBER: 139:301125
 TITLE: BAY-43-9006(Bayer/Onyx)
 AUTHOR(S): Lee, John T.; McCubrey, James A.
 CORPORATE SOURCE: Department of Microbiology and Immunology, Brody
 School of Medicine at East Carolina University,
 Greenville, NC, 27858-4353, USA
 SOURCE: Current Opinion in Investigational Drugs (Thomson
 Current Drugs) (2003), 4(6), 757-763
 CODEN: COIDAZ; ISSN: 1472-4472
 PUBLISHER: Thomson Current Drugs
 DOCUMENT TYPE: Journal; **General Review**
 LANGUAGE: English

*RM 301.
 27,
 C87*

AB A review. Bayer and Onyx are developing BAY-43-9006, an oral cytostatic
Raf kinase inhibitor for the potential treatment of colorectal and
 breast cancers, hepatocellular **carcinoma** and non-small-cell lung cancer,
 in addn. to acute myelogenous leukemia, myelodysplastic syndrome and other
 cancers. A US IND was filed in May 2000 and by Feb. 2003 BAY-43-9006 was
 in phase II trials, with phase III trials expected to begin later in 2003.
 REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS
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=>



chain nodes :

7 8 9 10 11

ring nodes :

1 2 3 4 5 12 13 14 15 16 17

chain bonds :

1-8 4-7 8-9 9-10 9-11 10-14

ring bonds :

1-2 1-5 2-3 3-4 4-5 12-13 12-17 13-14 14-15 15-16 16-17

exact/norm bonds :

1-2 1-8 4-7 8-9 9-10 9-11 10-14

exact bonds :

1-5 2-3 3-4 4-5

normalized bonds :

12-13 12-17 13-14 14-15 15-16 16-17

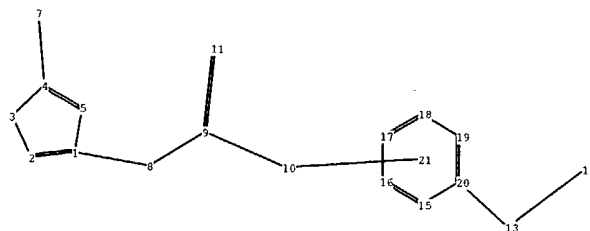
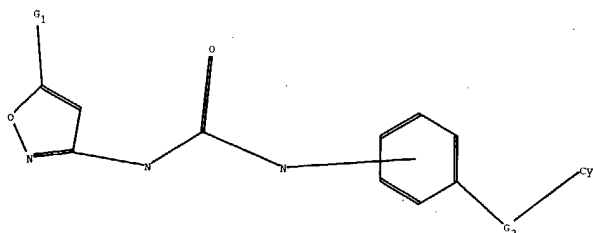
isolated ring systems :

containing 1 : 12 :

G1:cb,Ak

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom



chain nodes :

7 8 9 10 11 13 14

ring nodes :

1 2 3 4 5 15 16 17 18 19 20

chain bonds :

1-8 4-7 8-9 9-10 9-11 13-14 13-20

ring bonds :

1-2 1-5 2-3 3-4 4-5 15-16 15-20 16-17 17-18 18-19 19-20

exact/norm bonds :

1-2 1-8 4-7 8-9 9-10 9-11 13-14 13-20

exact bonds :

1-5 2-3 3-4 4-5

normalized bonds :

15-16 15-20 16-17 17-18 18-19 19-20

isolated ring systems :

containing 15 :

G1:Cb,Ak

G2:O,s

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS
13:CLASS 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:CLASS